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Space-time CFOSLS Methods with AMGe Upscaling

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Abstract This work considers the combined space-time discretization of time-dependent partial differential equations by using first order least square methods. We also impose an explicit constraint representing space-time mass conservation. To alleviate the restrictive memory demand of the method, we use dimension reduction via accurate element agglomeration AMG coarsening, referred to as AMGe upscaling. Numerical experiments demonstrating the accuracy of the studied AMGe upscaling method are provided.

1 Introduction

In this paper we explore a robust approach to derive combined space-time discretization methods for two classes (parabolic and hyperbolic) of time-dependent PDEs. We use the popular FOSLS (first order systems least-squares) approach (cf., e.g., Cai et al. [1994] or Carey et al. [1995])) treating time as an additional space variable and, in addition, we prescribe a space-time divergence equation as a constraint in order to maintain certain space-time mass conservation (following, e.g., Adler and Vassilevski [2014]).

More specifically, our approach is applied to the following model problem

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$$\frac{\partial S}{\partial t} + \operatorname{div}(\mathcal{L}(S)) = q_0(\mathbf{x}, t), \qquad \mathbf{x} \in \Omega \subset \mathbb{R}^d, t \in (0, T), \tag{1}$$

where $\mathcal{L}$ is at most a first-order differential operator with respect to the space variable $\mathbf{x}$ only. At $t = 0$ we impose an initial condition $S = S_0$ and on $\partial\Omega$ for all $t \in (0, T)$ we apply some appropriate boundary conditions (if any). More specifically we consider differential operators of the form

$$\mathcal{L}(S) := -k\nabla_\mathbf{x} S \quad \text{and} \quad \mathcal{L}(S) := f(S)\,\mathbf{u}(\cdot)$$

for respectively parabolic and hyperbolic problems, as explained in more details in Section 4 and 5.

2 Space-time Constrained First Order System Least Squares

Problem (1) can be rewritten as a first order system by introducing the "flux" variable $\boldsymbol{\sigma} := [\mathcal{L}(S); S]^\top$ as

$$\begin{aligned} \boldsymbol{\sigma} - \begin{bmatrix} \mathcal{L}(S) \\ S \end{bmatrix} &= 0, \\ \operatorname{div}_{\mathbf{x}, t} \boldsymbol{\sigma} \qquad &= q_0, \end{aligned} \tag{2}$$

where $\operatorname{div}_{\mathbf{x}, t}$ is the $d+1$-dimensional space-time divergence operator. We then introduce the FOSLS functional as

$$J(\boldsymbol{\sigma}, S) = \left\| \boldsymbol{\sigma} - \begin{bmatrix} \mathcal{L}(S) \\ S \end{bmatrix} \right\|_{0,\,K^{-1}}^2 + \| q_0 - \operatorname{div}_{\mathbf{x}, t} \boldsymbol{\sigma} \|_0^2,$$

where $K = K(\mathbf{x}) \in \mathbb{R}^{(d+1) \times (d+1)}$ is a symmetric and positive definite coefficient matrix and $\| \cdot \|_0$ ($\| \cdot \|_{0, K^{-1}}$) denotes the (weighted) $L_2(\Omega_T)$-norm with respect to the space-time domain $\Omega_T := \Omega \times (0, T)$. A constrained least-square version of (2) is given by minimizing the functional $J(\boldsymbol{\sigma}, S)$ under the constraint which is given by the conservation equation

$$(\operatorname{div}_{\mathbf{x}, t} \boldsymbol{\sigma}, w) = (q_0, w) \quad \text{for all} \quad w \in L_2(\Omega_T).$$

Here we denote with $(\cdot, \cdot)$ the inner product with respect to $L_2(\Omega_T)$. First order optimality conditions for the constrained minimization problem lead to the system of variational equations: Find $\boldsymbol{\sigma} \in H(\operatorname{div}_{\mathbf{x}, t}; \Omega_T)$, $S \in V$ and $\mu \in L_2(\Omega_T)$, such that

$$(\boldsymbol{\sigma}, \boldsymbol{\psi})_{K^{-1}} + (\operatorname{div}_{\mathbf{x},t} \boldsymbol{\sigma}, \ \operatorname{div}_{\mathbf{x},t} \boldsymbol{\psi}) - \left(\begin{bmatrix} \mathcal{L}(S) \\ S \end{bmatrix}, \ \boldsymbol{\psi} \right)_{K^{-1}} \qquad + (\mu, \ \operatorname{div}_{\mathbf{x},t} \boldsymbol{\psi}) = (q_0, \ \operatorname{div}_{\mathbf{x},t} \boldsymbol{\psi}),$$

$$-\left(\boldsymbol{\sigma}, \begin{bmatrix} \mathcal{L}(\phi) \\ \phi \end{bmatrix} \right)_{K^{-1}} \qquad\qquad + \left(\begin{bmatrix} \mathcal{L}(S) \\ S \end{bmatrix}, \begin{bmatrix} \mathcal{L}(\phi) \\ \phi \end{bmatrix} \right)_{K^{-1}} \qquad\qquad = 0,$$

$$(\operatorname{div}_{\mathbf{x},t} \boldsymbol{\sigma}, \ w) \qquad\qquad\qquad\qquad\qquad\qquad = (q_0, w)$$

$$\tag{3}$$

holds for all $\boldsymbol{\psi} \in H(\operatorname{div}_{\mathbf{x},t}; \Omega_T)$, all $\phi \in V$ and all $w \in L_2(\Omega_T)$. Here V denotes an appropriate function space for the unknown S, such that $\mathcal{L} : V \to L^2$ is a bounded operator. In a straightforward manner we obtain the finite element discretization of the CFOSLS system (3) by using appropriate finite dimensional spaces, i.e. we use $\boldsymbol{\sigma}_h \in \mathbf{R}_h \subset H(\operatorname{div}_{\mathbf{x},t}; \Omega_T), S_h \in V_h \subset V$ and $\mu_H \in W_H \subset L_2(\Omega_T)$. Note that the Lagrangian multiplier μ_H belongs to the space W_H of discontinuous piecewise polynomials defined on a coarser mesh $\mathcal{T}_H$ (the lowest order being piecewise constants). The fine mesh $\mathcal{T}_h$ is constructed by performing one uniform refinement of $\mathcal{T}_H$. This choice leads to a *relaxed* Petrov-Galerkin discretization of the mass conservation equation and prevents overconstraining the resulting system. A relevant error analysis of the above discretization has been presented in Adler and Vassilevski [2014]. Finally, using appropriate basis functions for the discrete functions spaces, we obtain the system of linear equations for the saddle point problem

$$\begin{bmatrix} A & B^\top & D^\top \\ B & C & 0 \\ D & 0 & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\sigma}_h \\ \mathbf{S}_h \\ \boldsymbol{\mu}_H \end{bmatrix} = \begin{bmatrix} f_h \\ 0 \\ g_H \end{bmatrix}. \tag{4}$$

3 AMGe Upscaling

The AMGe (element agglomeration) coarsening has been developed at LLNL, originally to derive hierarchies of finite element spaces for designing multigrid solvers for bilinear forms corresponding to an entire de Rham sequence of spaces (H^1-conforming, $H(\operatorname{curl})$-conforming, and $H(\operatorname{div})$-conforming), (Pasciak and Vassilevski [2008]), and more recently (Lashuk and Vassilevski [2012, 2014]) to ensure that these hierarchies of spaces have guaranteed approximation properties. Such spaces are hence suitable to construct accurate coarse discretizations and can be used as a tool for dimension reduction, also refereed to as numerical upscaling.

The CFOSLS space-time discretization approach leads to saddle–point systems involving function spaces in the divergence constraint that are $H(\operatorname{div})$-conforming. This allows to solve combined space-time problems up to 2 space dimensions using the existing AMGe upscaling framework for 3D Raviart-Thomas elements. The goal in the near future is to extend this framework to 4D Raviart-Thomas analogs. This paper, as a first step, demonstrates the feasibility of the AMGe upscaling approach applied to combined space-time

discretization that is both accurate, mass-conservative and achieving reasonable dimension reduction, which makes the expensive direct space-time approach (applied on the fine grid) feasible at coarser upscaled levels.

In the next sections we study the presented approach in detail for the two differential operators introduced in the beginning of this work. The finite element library MFEM (MFEM) is used to assemble the discretized systems which are then solved using the algebraic multigrid solvers (AMG) in hypre (HYPRE).

4 Parabolic problem

Here we choose the differential operator $\mathcal{L}(S) := -k\nabla_{\mathbf{x}}S$, where $k = k(\mathbf{x})$ is a given positive coefficient. For simplicity, we use homogeneous Dirichlet boundary conditions on $\partial\Omega$ for all $t \in (0, T)$. For the variational problem (3) we then introduce the weight

$$K = \begin{bmatrix} kI_d & 0 \\ 0 & 1 \end{bmatrix}.$$

A natural space for the unknown S is then given by $V = L_2(0, T, H_0^1(\Omega))$. For the discretization, we use a standard conforming subspace $V_h \subset V$ consisting of piecewise Lagrangian polynomials which are globally continuous. We then solve the discretized saddle-point problem (4) by using the MINRES method with the block diagonal preconditioner

$$\hat{P} = \begin{bmatrix} \hat{A} & 0 & 0 \\ 0 & \hat{C} & 0 \\ 0 & 0 & \hat{W} \end{bmatrix},$$

where $\hat{A}$ denotes the auxiliary space AMG solver for $H(\text{div})$-problem applied to the matrix A (HypreADS, Kolev and Vassilevski [2012]), $\hat{C}$ is a standard AMG preconditioner for C (BoomerAMG, HYPRE), and $\hat{W}$ represents the diagonal of the $L_2(\Omega_T)$ mass matrix W.

Example 1. In this example we let $\Omega = (0, 1)^2$, $T = 1$ and $k \equiv 1$. The exact solution is given by $u(x_1, x_2, t) = e^{-t}\sin(\pi x_1)\sin(\pi x_2)$.

The initial – fine – space-time mesh (level 0) is an unstructured tetrahedral mesh with $490, 200$ elements. We use graph partitioning algorithms (Karypis and Kumar [1998]) to construct the agglomerated space-time meshes shown in Figure 1. For the discretization, we use lowest order finite element spaces on the fine grid and then we construct the hierarchy of coarse spaces as explained in Section 3. Table 1 reports the errors with respect to the exact solution. We observe that the upscaling procedure allows to dramatically reduce the

number of unknowns maintaining reasonable good approximations, see also Figure 1.

level	elements	dof	$\|S - S_H\|_0$	$\|\boldsymbol{\sigma} - \boldsymbol{\sigma}_H\|_0$	$\|u_h - u_H\|_0$	$\|\boldsymbol{\sigma}_h - \boldsymbol{\sigma}_H\|_0$	iter
0	490,200	1,579,808	3.4360E-03	2.4217E-02	-	-	107
1	7,700	218,089	6.2509E-03	3.2351E-02	2.0985E-03	3.5408E-02	80
2	1,043	59,085	2.5489E-02	7.5482E-02	8.3829E-03	1.0854E-01	102
3	179	12,366	8.1318E-02	1.7308E-01	2.6544E-02	2.5752E-01	60
4	39	3,127	2.3470E-01	3.7018E-01	7.6846E-02	5.5365E-01	34
5	8	635	3.0685E-01	5.1457E-01	1.0064E-01	7.7024E-01	27

Table 1 Numerical errors for different agglomeration levels for Example 1.

5 Hyperbolic problem

Here we consider the differential operator $\mathcal{L}(S) := f_0(S_*)S\,\mathbf{u}(\cdot)$, with the given velocity field $\mathbf{u}$ (satisfying $\mathbf{u} \cdot \mathbf{n_x} = 0$ on $\partial\Omega$) and the given positive function $f_0 = f_0(S_*)$. Such equations can be used, for example, to model the evolution in time of water or gas saturation in an oil reservoir. We then introduce the weight

$$K = K(S_*) = \begin{bmatrix} f_0(S_*)I_d & 0 \\ 0 & 1 \end{bmatrix} \quad \text{which gives} \quad \boldsymbol{\sigma} = K(S_*) \begin{bmatrix} \mathbf{u} \\ 1 \end{bmatrix} S.$$

A natural setting for S is given by $V = L_2(\Omega_T)$. Using the second equation of (3) we can eliminate the unknown S and we obtain the reduced system for $\boldsymbol{\sigma}$ and the Lagrange multiplier μ: Find $\boldsymbol{\sigma} \in H(\mathrm{div}; \Omega_T)$ and $\mu \in L_2(\Omega_T)$, such that

$$\left(\left(K^{-1} - \delta_K^{-1} \begin{bmatrix} \mathbf{u} \\ 1 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ 1 \end{bmatrix}^\top \right) \boldsymbol{\sigma}, \, \boldsymbol{\psi} \right) + (\mu, \mathrm{div}\,\boldsymbol{\psi}) = 0, \qquad (5)$$
$$(\mathrm{div}\,\boldsymbol{\sigma}, w) = (q, w)$$

holds for all $\boldsymbol{\psi} \in H(\mathrm{div}; \Omega_T)$ and for all $w \in L_2(\Omega_T)$. Here $\delta_K \in \mathbb{R}$ is given by

$$\delta_K = \begin{bmatrix} \mathbf{u} \\ 1 \end{bmatrix}^\top K \begin{bmatrix} \mathbf{u} \\ 1 \end{bmatrix} \qquad \text{and further} \qquad S = \delta_K^{-1} \begin{bmatrix} \mathbf{u} \\ 1 \end{bmatrix}^\top \boldsymbol{\sigma}.$$

It can be shown that the matrix $K^{-1} - \delta_K^{-1} \begin{bmatrix} \mathbf{u} \\ 1 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ 1 \end{bmatrix}^\top$ in (5) is positive definite on the nullspace of the divergence operator, if $\mathrm{div}_\mathbf{x}(f_0(S_*)\mathbf{u}) \geq 0$ in Ω and $\mathbf{u} \cdot \mathbf{n_x} = 0$ on $\partial\Omega$.

Numerical solution S_h Numerical solution $|\boldsymbol{\sigma}_h|$ Agglomerated mesh on level 0

Numerical solution S_h Numerical solution $|\boldsymbol{\sigma}_h|$ Agglomerated mesh on level 1

Numerical solution S_h Numerical solution $|\boldsymbol{\sigma}_h|$ Agglomerated mesh on level 2

Numerical solution S_h Numerical solution $|\boldsymbol{\sigma}_h|$ Agglomerated mesh on level 3
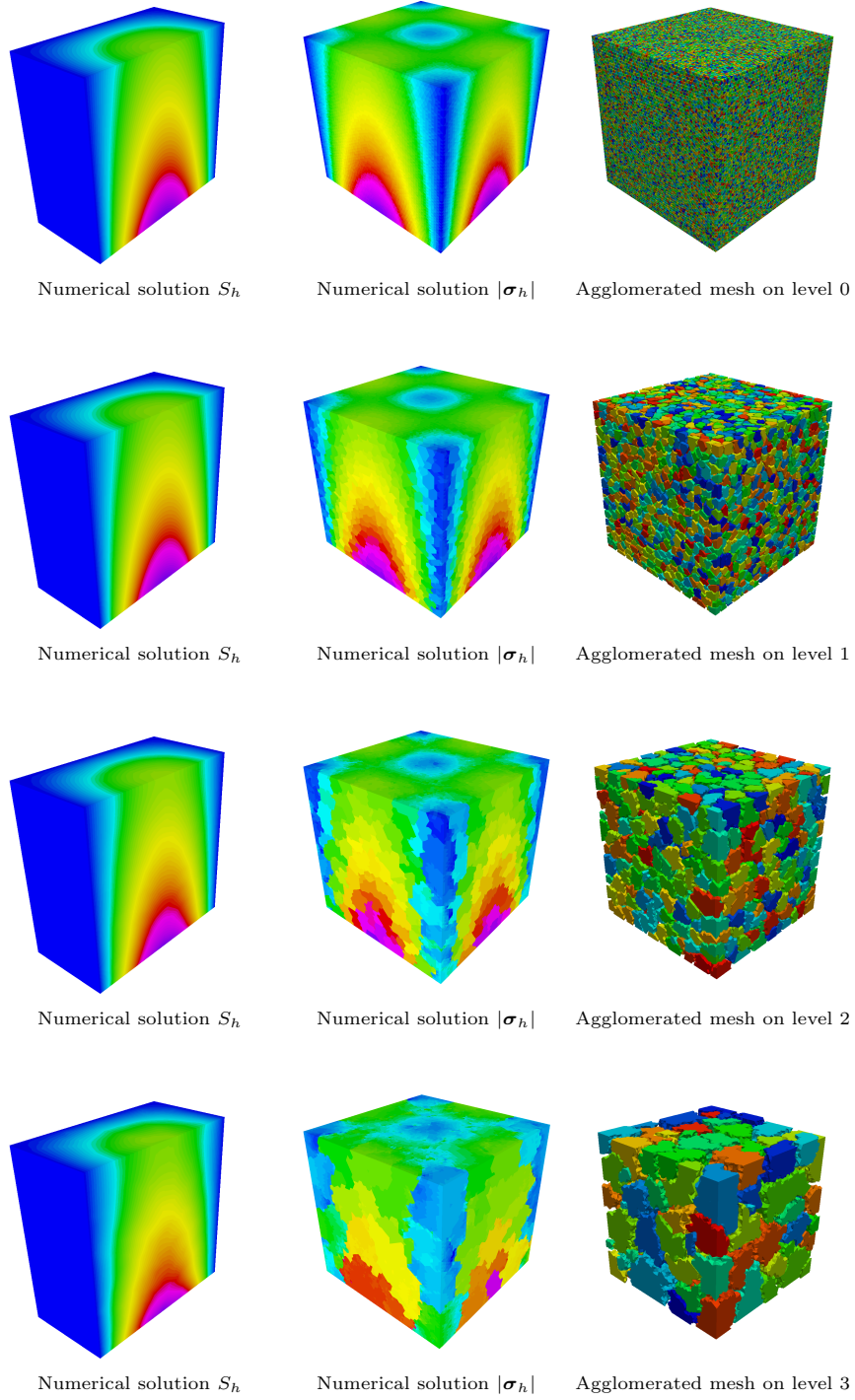
Fig. 1 Numerical solutions and agglomerated meshes for different levels (Example 1).

Example 2. In this example we consider $\Omega = \{\mathbf{x} \in \mathbb{R}^2 : |\mathbf{x}| < 1\}$, $T = 2$, $f_0(S_*) \equiv 1$ and $q_0 \equiv 0$ with the velocity function and the initial condition

$$\mathbf{u}(x_1, x_2, t) = \begin{bmatrix} -x_2 \\ x_1 \end{bmatrix} \quad \text{and} \quad S_0(x_1, x_2) = e^{-100[(x_1-0.5)^2 + x_2^2]}.$$

For the discretization we use Raviart-Thomas pairs $\mathbf{R}_h, W_h$ for $\boldsymbol{\sigma}$ and the Lagrange multiplier μ. The initial fine mesh (an unstructured tetrahedral mesh with $1,315,708$ elements) and the agglomerated meshes are shown in Figure 2. Table 2 shows (similarly to what already observed for the parabolic example) that upscaling allows to achieve both effective dimension reduction and good approximation of the fine grid solution (level 0). The divergence free solver Christensen et al. [2015] allows for the robust solution of the discretized saddle point problem at each level as shown by the number of iterations reported in Table 2.

level	elements	dof	$\|\boldsymbol{\sigma}_h - \boldsymbol{\sigma}_H\|_0$	$\|\mu_h - \mu_H\|_0$	iter
0	1,315,708	3,970,948	-	-	39
1	164,495	1,636,016	1.1665E-03	1.2176E-09	39
2	21,009	495,815	5.0647E-03	2.2788E-04	33
3	3,215	99,004	9.1879E-03	4.6800E-04	24
4	684	22,324	1.0483E-02	5.6677E-04	19
5	200	8,041	1.2115E-02	7.1052E-04	16

Table 2 Numerical errors for different agglomeration levels for Example 2.

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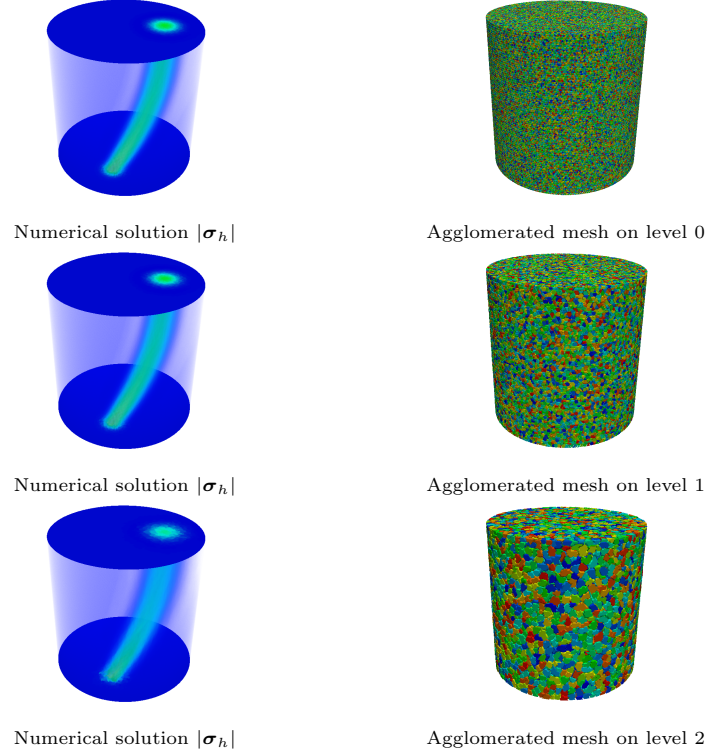
| Numerical solution $|\boldsymbol{\sigma}_h|$ | Agglomerated mesh on level 0 |

| Numerical solution $|\boldsymbol{\sigma}_h|$ | Agglomerated mesh on level 1 |

| Numerical solution $|\boldsymbol{\sigma}_h|$ | Agglomerated mesh on level 2 |

Fig. 2 Numerical solution and agglomerated meshes for different levels (Example 2).

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